METABOLOME PROFILING METHODS USING CHROMATOGRAPHIC AND SPECTROSCOPIC DATA IN PATTERN RECOGNITION ANALYSIS

ABSTRACT

Methods are provided that apply neural network technology to recognize small metabolic changes in microorganisms, plants or animals to detect changes induced by pesticide (herbicide, insecticide, fungicide) treatment, genetic modification, environmental stress, and other external or internal factors that have influence on metabolite concentrations. The method implements recognition of nuclear magnetic resonance spectra, mass spectra, and/or chromatograms of crude plant extracts and association of such spectra or chromatograms with the treatment of tissue before harvest. The spectra and chromatograms have information of all the metabolites above a concentration threshold contained in the plant tissue extract. The method applies mathematical models to the very complex plant tissue extract and allows the detection of treatments with bioregulators such as pesticides, or genetic modifications such as gene insertions or deletions.

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